meso-Hexestrol

84-16-2 | DTXSID2022381

Model Performance

Model	Data	
IVIOGEI	Dala	

Weighted KNN model

5-fold CV ((75%)	Training (75%)	Test (25%	·)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 55.1

Global applicability domain: Inside

Local applicability domain index: 4.06e-01

Confidence level: 6.81e-01

Nearest Neighbors from the Training Set

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Disulfoton Measured: 219 Predicted: 151 Image not found

Iprobenfos Measured: 8.71 Predicted: 4.13 Image not found

Bis(pentamethylenethiuram)tetrasulfide

Measured: 17.0 Predicted: 21.1

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Isoamyl ether Measured: 170 Predicted: 137 Image not found

Parathion
Measured: 97.7
Predicted: 22.3